

2-(Methylsulfanyl)quinoxaline
21948-73-2 | DTXSID00325902

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.24

Global applicability domain: Inside

Local applicability domain index: 5.30e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

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4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69

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Triethylamine

Measured: 4.90

Predicted: 5.95

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N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 52.5

Predicted: 17.5

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Methyl tert-butyl ether

Measured: 1.51

Predicted: 3.67

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6-Nitrobenzimidazole

Measured: 2.51

Predicted: 3.81